Procedure for Estimation and Reporting of Discretization Error in CFD Applications

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Since 1990, the Fluids Engineering Division of ASME has pursued activities concerning the detection, estimation and control of numerical uncertainty and/or error in computational fluid dynamics (CFD) studies. The first quality-control measures in this area were issued in 1986 (Roache et al., [8]), and revised in 1993 (Freitas [5]). Given the exponential increase in CFD related publications, and the many significant advancements in computational techniques and computer technology, it has become necessary to revisit the same issue and formulate a more detailed policy to further improve the quality of publications in this area. This brief note provides specific guidelines for prospective authors for calculation and reporting of discretization error estimates in CFD simulation for experimental data may or may not be available for comparison. The underlying perspective is that CFD-related studies will eventually aim to predict the outcome of a physical event for which experimental data is not available.

It should be emphasized that the requirements outlined in this note do not preclude those already published in the previous two policy statements (Roache et al. [8], Freitas [5]). It is also important to keep in mind that the procedure recommended in this note cannot possibly encompass all possible scenarios or applications.

Preliminaries

The ***computer code*** used for an application must be fully referenced, and previous ***verification studies*** must be briefly described. The word "verification" is used in this note in its broadest sense, meaning that the computer code is capable of solving a system of non-linear coupled partial differential equations with a properly posed set of initial and/or boundary conditions correctly, and reproduces the exact solution to these equations when sufficiently fine grid resolution (both in time and space) is employed. The ***formal order of accuracy*** in time and space for each equation solved should be also stated clearly, with proper references where this information is accessible to the readers. Before any discretization error estimation is calculated, it must be ensured that ***iterative convergence*** (if iterative methods are used) is achieved with at least three orders of magnitude decrease in the normalized residuals for each equation solved. For time-dependent problems, iterative convergence at every time step should be checked, and sample convergence trends should be documented for selected, critically important, variables.

The recommended method for discretization error estimation is the Richardson extrapolation (RE) method. Since its first elegant application by its originator (Richardson [6] [7]), this method has been studied by many authors. Its intricacies, shortcomings and generalization have been widely investigated. A short list of references given in the bibliography ([2,3,4,5,9,10,11]) is selected for the direct relevance of these references to the subject and for brevity. The RE method is far from being perfect. The local RE values of predicted variables may not exhibit a smooth, monotonic dependence on grid resolution, and in a time-dependent calculation, this non-smooth response will also be a function of time and space. Nonetheless, it is currently the most robust method available for the prediction of numerical uncertainty. Prospective authors can find many examples in the above references. As new and more reliable methods emerge, the present policy statement should be re-assessed and modified as needed, say every five years interval.

The GCI method described herein is an acceptable and recommended method that has been evaluated over several hundred CFD cases. If authors choose to use it, the method per se will not be challenged in the paper review process. If authors choose to use another method, its adequacy will be judged in the review process. This policy is not meant to discourage further development of new methods; in fact, JFE encourages the development and statistically significant evaluation of alternative methods of estimation of error and uncertainty. Rather, this policy is meant to facilitate CFD publication by providing practitioners with a method that is straightforward to apply, is fairly well justified and accepted, and will avoid possible review bottlenecks, especially when the CFD paper is an applications paper rather than one concerned with new CFD methodology.

Recommended Procedure for estimation of discretization error

Step 1 Define a representative cell, mesh or grid size h. For example for three-dimensional calculations

$$h = \left[\frac{1}{N} \sum_{i=1}^{N} (\Delta V_i) \right]^{1/3} . \qquad \textbf{(1)}$$

For two-dimensions,

$$h = \left[\frac{1}{N} \sum_{i=1}^{N} (\Delta A_i) \right]^{1/2} \qquad (2)$$

where ΔV_i is the volume and ΔA_i is the area of the i^{th} cell, and N is the total number of cells used for the computations. Eqs. (1) and (2) are to be used when integral quantities, e.g., drag coefficient is considered. For field variables, the local cell size can be used. Clearly, if an observed global variable is used, it is then appropriate to use also an average "global" cell size.

Step 2 Select three significantly different set of grids, and run simulations to determine the values of key variables important to the objective of the simulation study, for example, a

variable ϕ critical to the conclusions being reported. It is desirable that the grid refinement factor, $r=h_{coarse}/h_{fine}$, be greater than 1.3. This value of 1.3 is based on experience, and not on formal derivation. The grid refinement should, however, be done systematically, that is, the refinement itself should be structured even if the grid is unstructured. Use of geometrically similar cells are preferable.

Step 3 Let $h_1 < h_2 < h_3$ and $r_{21}=h_2/h_1$, $r_{32}=h_3/h_2$, and calculate the apparent order, p, of the method using the expression

$$p = \frac{1}{\ln(r_{21})}\left|\ln|\varepsilon_{32}/\varepsilon_{21}| + q(p)\right| , \tag{3a}$$

$$q(p) = \ln\left(\frac{r_{21}^{p} - s}{r_{32}^{p} - s}\right) , \tag{3b}$$

$$s = 1 \cdot \mathrm{sign}(\varepsilon_{32}/\varepsilon_{21}) , \tag{3c}$$

where $\varepsilon_{32}=\phi_3-\phi_2$, $\varepsilon_{21}=\phi_2-\phi_1$, ϕ_k denoting the solution on the k^{th} grid. Note that $q(p)=0$ for $r=const.$ Eq. (3) can be solved using fixed-point iteration, with the initial guess equal to the first term. The absolute value in Eq. (3a) is necessary to ensure extrapolation towards $h=0$ (Celik & Karatekin [3]). Negative values of $\varepsilon_{32}/\varepsilon_{21}<0$ are an indication of oscillatory convergence. If possible, the percentage occurrence of oscillatory convergence should also be reported agreement of the observed apparent order with the formal order of the scheme used can be taken as a good indication of the grids being in the asymptotic range; the converse should not necessarily be taken as a sign of unsatisfactory calculations. It should be noted that if either $\varepsilon_{32}=\phi_3-\phi_2$ or $\varepsilon_{21}=\phi_2-\phi_1$ is "very close" to zero, the above procedure does not work. This might be an indication of oscillatory convergence or, in rare situations, it may indicate that the "exact" solution has been attained. In such cases, if possible, calculations with additional grid refinement may be performed; if not, the results may be reported as such.

Step 4 Calculate the extrapolated values from

$$\phi_{ext}^{21} = (r_{21}^{p}\phi_1 - \phi_2)/(r_{21}^{p} - 1) ; \tag{4}$$

Similarly, calculate ϕ_{ext}^{32} .

Step 5 Calculate and report the following error estimates, along with the apparent order p:

Approximate relative error:

$$e_a^{21} = \left|\frac{\phi_1 - \phi_2}{\phi_1}\right| , \tag{5}$$

Extrapolated relative error:

$$e_{ext}^{21} = \left| \frac{\phi_{ext}^{12} - \phi_1}{\phi_{ext}^{12}} \right| , \quad (6)$$

The fine grid convergence index:

$$\mathrm{GCI}_{\mathrm{fine}}^{21} = \frac{1.25 e_a^{21}}{r_{21}^p - 1} , \quad (7)$$

Table 1 illustrates this calculation procedure for three selected grids. The data used is taken from Celik & Karatekin [3]), where the turbulent two-dimensional flow over a backward facing step was simulated on non-uniform structured grids with total number of cells N_1, N_2, and N_3. Hence, according to Table 1, the numerical uncertainty in the fine-grid solution for the reattachment length should be reported as 2.2%; note this does not account for modeling errors.

Table 1: Sample calculations of discretization error

	ϕ = dimensionless reattachment length (*with monotonic convergence*)	ϕ = axial velocity at x/H=8, y=0.0526 (p < 1)	ϕ = axial velocity at x/H=8, y=0.0526 (*with oscillatory convergence*)
N_1, N_2, N_3	18000, 8000, 4500	18000, 4500, 980	18000, 4500, 980
r_{21}	1.5	2.0	2.0
r_{32}	1.333	2.143	2.143
ϕ_1	6.063	10.7880	6.0042
ϕ_2	5.972	10.7250	5.9624
ϕ_3	5.863	10.6050	6.0909
p	1.53	0.75	1.51
ϕ_{ext}^{21}	6.1685	10.8801	6.0269
e_a^{21}	1.5%	0.6%	0.7%
e_{ext}^{21}	1.7%	0.9%	0.4%
GCI_{fine}^{21}	2.2%	1.1%	0.5%

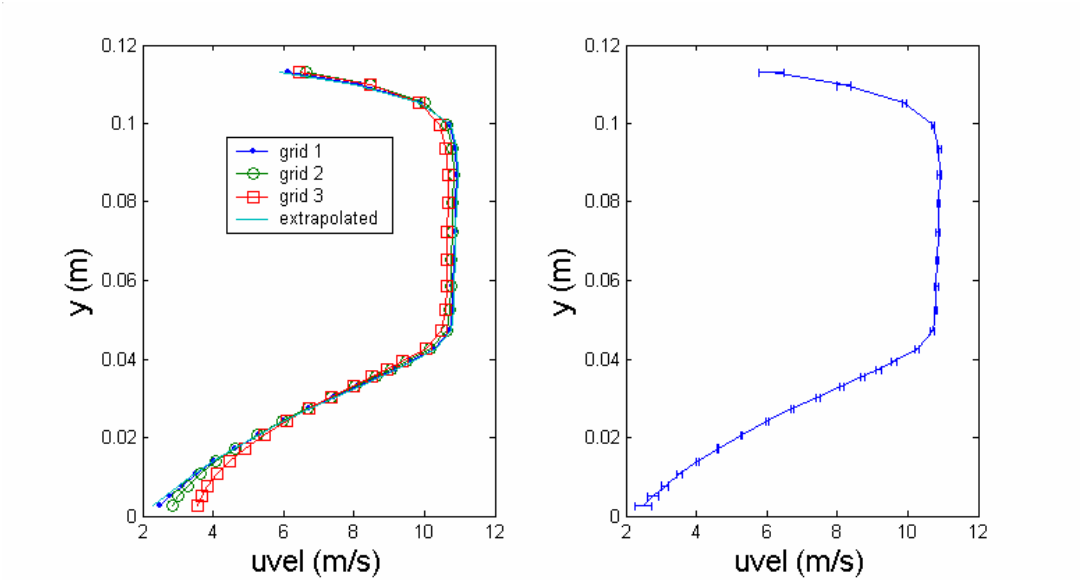
Discretization Error Bars

When computed profiles of a certain variable are presented, it is recommended that numerical uncertainty is indicated by error bars on the profile, analogous to experimental uncertainty. It is

further recommended that this be done using the GCI in conjunction with an average value of $p=p_{ave}$ as a measure of the global order of accuracy. This is illustrated in Figs. 1 and 2.

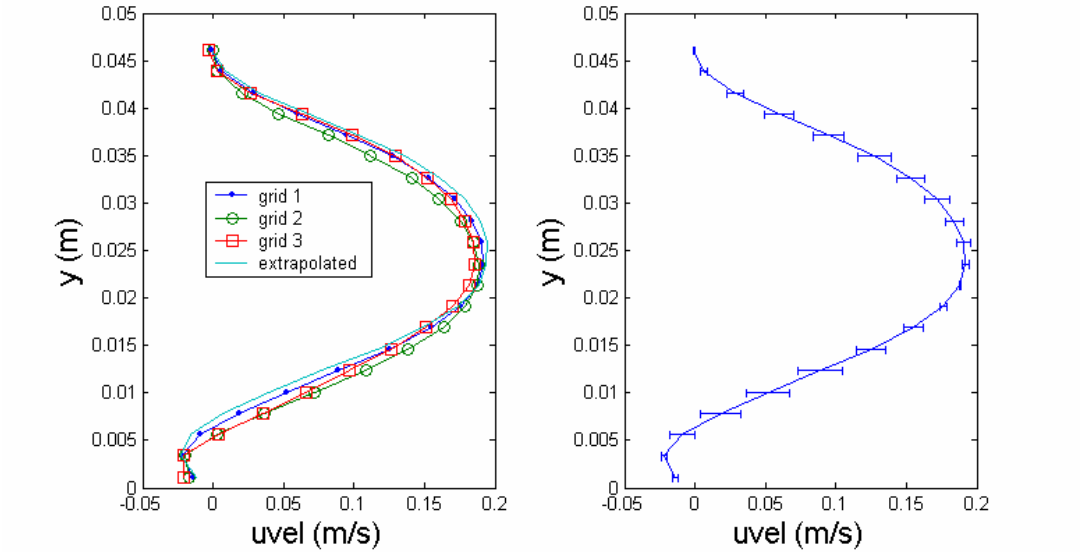
Figure 1 (data taken from Celik & Karatekin [3]) presents an axial velocity profile along y-axis at an axial location of x/H=8.0 for a *turbulent* two-dimensional backward-facing-step flow. The three sets of grids used were 980, 4500, and 18000 cells, respectively. The local order of accuracy p calculated from Eq. (3) ranges from 0.012 to 8.47, with a global average p_{ave} of 1.49, which is a good indication of the hybrid method applied for that calculation. Oscillatory convergence occurs at 20% of the 22 points. This averaged apparent order of accuracy is used to assess the GCI indices values in Eq. (7) for individual grids, which is plotted in the form of error bars, as shown in Fig. 1(b). The maximum discretization uncertainty is 10%, which corresponds to ±0.35 m/s.

Figure 2 (data taken from Celik & Badeau [1]) presents an axial velocity profile along the y-axis at the station x/H=8.0 for a *laminar* two-dimensional backward-facing-step flow. The Reynolds number based on step height is 230. The sets of grids used were 20x20, 40x40, and 80x80, respectively. The local order of accuracy p ranges from 0.1 to 3.7, with an average value of p_{ave} = 1.38. In this figure, 80% out of 22 points exhibited oscillatory convergence. Discretization error bars are shown in Fig. 2(b), along with the fine-grid solution. The maximum discretization error was about 100%; this high value is relative to a velocity near zero, and corresponds to a maximum uncertainty in velocity of about ±0.012 m/s.



(a) (b)

Figure 1(a): Axial velocity profiles for a two-dimensional turbulent backward-facing-step flow calculation, Ref: Celik & Karatekin [1];
(b): Fine-grid solution, with discretization error bars computed using Eq. (7).



(a) (b)

Figure 2(a): Axial velocity profiles for a two-dimensional laminar backward-facing-step flow calculation, Ref: Celik & Badeau [1];
(b): Fine-grid solution, with discretization error bars computed using Eq. (7).

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